

HLWYM HEmails

From: [REDACTED]
Sent: Tuesday, November 09, 1999 6:51 AM
To: Roberto Pabalan <rpabalan@swri.edu>; [REDACTED]; hwstock@sandia.gov
Cc: dpickett@swri.edu
Subject: Re:Fwd:Re: geochemistry calculations
Attachments: RFC822.TXT

Follow Up Flag: Follow up
Flag Status: Flagged

Hi --

I placed the CD contents on the following location:
<http://garnet.energylan.sandia.gov/~ymp/>

This address points to a public Outbox on a secure system. The best way to access the site is probably through your browser; just click on the link above, then select directory Pu-ceram_CD. The directories correspond to those in the Pu-ceram report attachment.

I tried to transfer most files as binary, but some of the text files may have been futzed with by the ftp client. The best way to view the *.elem_???.txt files is to drop them onto Excel. With the *.6i and *.6o files, you should have a pretty complete set of results.

That FTP server will soon run out of room, so if you really want to see the files, you should check them out in the next week, before I clean the system.

The binaries (*.bin files) are large; however, they provide the best way to explore the chemistry of the test cases. To view them, you will need to download pp.exe, prefer.pp, help_pp, external.fnt and the associated files into a directory on a Win95, Win98 or Win3.1x machine. Load the binary you wish to see into that directory, open a DOS box into that directory, and invoke the program:

```
pp /4 myfile.bin
```

where myfile.bin is the name of the particular binary. If the screen gets garbage, use the command line pp 6 /4 myfile.bin

to enforce low-res VGA mode.

There is an old manual for the PP program in <http://garnet.energylan.sandia.gov/~ymp/eq/PP.doc> . Since you won't have the proper environment variables set, the only way to use the "What is this?" capability would be to copy the data0 file of choice to data0.com, within the same directory.

On multiflo: we wanted to use that code. Bob MacKinnon did the legwork, but the paperwork inertia was far too great, and qualification looked really complicated, since there were few tests cases available, and the range of capabilities is so large. Since TOUGHREACT is already qualified, it would be very hard to push for qualification of a similar code.

Roberto Pabalan <rpabalan@swri.edu> said:

> Harlan:

>

> Thank you for your quick reply to David's questions. I find your work

presented

> in the Pu-ceramic report very interesting. We have initiated new
> activities--modeling and experimental--designed to provide a better
> understanding of the chemistry of water inside corroding waste
> packages. We

may

> take a similar approach of using EQ3/6 in the calculations, perhaps
supplemented

> by reactive transport calculations with MULTIFLO and coupled
corrosion/transport

> calculations with TECTRAN (currently proprietary, funded by GRI).

>

> I would appreciate receiving a copy of the electronic data for EQ6
calculations,

> mainly for benchmarking our calculations. At some point, we would also

> be interested in getting a copy of the YMP-qualified EQ3/6 database,

> either

through

> you or from Tom/Jim or Dave Sassani.

>

> You can try sending a copy of the electronic data via ftp to
ftp.swri.edu/pub.

> Please advise me if you were able to do so--I'll retrieve the file

> right

away to

> free up the disk space. However, I'm not sure if there is enough room

> for

600

> MB.

>

> Thanks.

>

> bobby pabalan

> _____Reply Separator_____

> Subject: Fwd:Re: geochemistry calculations

> Author: David Pickett

> Date: 11/8/99 5:38 PM

>

> Bobby - Reply from Stockman.

>

> David

>

> _____Forward Header_____

> Subject: Re: geochemistry calculations

> Author: "H.W. Stockman" [REDACTED]

> Date: 11/8/99 3:39 PM

>

>

> ----- Original Message -----

> From: David Pickett <dpickett@swri.edu>

> To: [REDACTED]

> Sent: Monday, November 08, 1999 1:44 PM

> Subject: geochemistry calculations

>

>

>>

> > Harlan,
> >
> > Thanks again for the report you sent several weeks ago. Bobby
> > Pabalan is
> > the
> > lead here on near field issues, and he was wondering if there are
> > similar reports available for related calculations having to do with
> > in-package or in-drift chemistry (more generally than just related
> > to criticality). I
> > realize
> > that is a rather open-ended question, but I would appreciate any
> > suggestions you
> > might have. We're not so much interested in the results and
> > conclusions as
> > we
> > are in getting a better idea of how DOE plans to do this type of
> > work in
> > the
> > future.
>
> > Actually, we should have some pretty good examples soon. JP Nicot
> > qualified PHREEQC, and is completing a set of calculations on
> > U-silicate precipitation in fractures. He sent up some rather
> > interesting plots this morning, with calculations of soddyite
> > precipitation over a 250 meter path, and I believe he is writing up
> > the discussion now. We will have the draft of our Pu-ceramic external
> > criticality report out in early January, and assuming it is "legal"
> > and my
> > bosses agree, I can send results of intermediate work by the end of November.
>
> > We have broadened our work to include more realistic models, and more
> > sensitivity studies. There are still substantial uncertainties in the
> > effective surface area for the near field calculations
>
> > We are going to rerun many of our calculations with a new thermo
> > database soon, and it might be appropriate to wait for the comparison
> > between old and new.
> > We are in the process of getting a single EQ6 database qualified for
> > use at YMP. Paul Cloke arranged meetings with Dave Sassani, the DOE
> > reps, Tom Wolery and Jim Johnson of LLNL, Wolfgang Runde of LANL, and
> > various M&O folks to hammer out a sensible and defensible data set.
> > Johnson and Sassani are plugged into the Helgeson-derived datasets, so
> > we have some academic credibility. Sensitive issues that we wish to
> > resolve
> > include:
> > the stability of Pu carbonate complexes; methods of calculating
> > activity coefficients for the Pu carbonate species; and the current
> > uncertainty in U-silicate data.
>
> > > He also asked about a set of data cited in your Pu ceramic report as
> > > CRWMS
> > > M&O
> > > 1999: "Electronic data for EQ6 calculations...." Is that available?
>
> > It is. As a CD, it is about 600 MB, but most of that is in the binary
> > files, which we use only for graphing data (the graphing software is

> included on the CD). I can either cut a copy of the CD, or I can put
> the files on an FTP server (I think the latter makes more sense; do
> you have an FTP site not within a firewall?). I'll forward this note
> to myself at work; but if you don't hear from me in a day, send a
> gentle reminder.

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Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 544

Mail Envelope Properties ([REDACTED] 19991109065100)

Subject: Re:Fwd:Re: geochemistry calculations
Sent Date: 11/9/1999 6:51:00 AM
Received Date: 11/9/1999 6:51:00 AM
From: [REDACTED]

Created By: [REDACTED]

Recipients:

"dpickett@swri.edu" <>
Tracking Status: None
"Roberto Pabalan <rpabalan@swri.edu>" <>
Tracking Status: None
[REDACTED] <>
Tracking Status: None
"hwstock@sandia.gov" <>
Tracking Status: None

Post Office:

Files	Size	Date & Time
MESSAGE	6778	11/9/1999 6:51:00 AM
RFC822.TXT	1108	

Options

Priority: Standard
Return Notification: No
Reply Requested: No
Sensitivity: Normal
Expiration Date:
Recipients Received: Follow up

Received: from watchtower.cnwra.swri.edu by mail.cnwra.swri.edu (ccMail Link to SMTP R8.10.00)
; Tue, 09 Nov 99 13:48:44 -0600
Return-Path: <nobody@jubjub.wizard.com>
Received: from trapdoor.cnwra.swri.edu by watchtower.cnwra.swri.edu (4.1/SMI-4.1)
id AA11220; Tue, 9 Nov 99 13:50:35 CST
Received: from swri.edu (swri.edu [129.162.26.41])
by trapdoor.cnwra.swri.edu (8.8.7/8.8.7) with ESMTP id NAA04044;
Tue, 9 Nov 1999 13:51:08 -0600 (CST)
Received: from jubjub.wizard.com (jubjub.wizard.com [209.170.216.9])
by swri.edu (8.9.3/8.9.3) with ESMTP id NAA21038;
Tue, 9 Nov 1999 13:51:24 -0600 (CST)
Received: (from nobody@localhost) by jubjub.wizard.com (8.9.3/8.6.9) id LAA90982; Tue, 9 Nov 1999
11:51:08 -0800 (PST)
Date: Tue, 9 Nov 1999 11:51:08 -0800 (PST)
Message-Id: <199911091951.LAA90982@jubjub.wizard.com>
To: Roberto Pabalan <rpabalan@swri.edu>, [REDACTED],
hwstock@sandia.gov
Subject: Re:Fwd:Re: geochemistry calculations
From: [REDACTED]
X-Mailer: TWIG 1.0.1
Cc: dpickett@swri.edu